Transient CFD: How Valuable is It for Catalyst Design?

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ABSTRACT

The design of the hot-end exhaust system dictates the performance of the exhaust system in terms of emissions, power loss and durability. The engine-out flow is highly transient and hot, and may place tremendous thermal and inertial loads on a catalyst. Therefore, time-dependent and detailed flow and thermal field simulation may be crucial. This study is geared towards assessing the value of transient flow simulations for close-coupled and underbody converters. For this purpose key parameters are defined and compared for similar sized close-coupled and underbody catalysts via transient and steady flow simulations.

INTRODUCTION

The flow distribution within the exhaust manifold and catalytic converter dictates the performance of the exhaust system in terms of emissions, power loss and durability. The engine-out flow is highly transient and hot, and may place tremendous thermal and inertial loads on a catalyst. Such thermal and pressure loadings are known to result in durability problems such as brick and/or mat erosion even structural failure. Even without durability issues, flow information is required for ensuring emission conversion capability of a converter. Therefore, time-dependent and detailed flow and thermal field information may be crucial for catalysts. More critical is determining the way this information is digested and reflected on the designs. This study aims to condense the vast flow information from a transient numerical analysis and utilize key parameters to define our understanding of catalyst performance and durability issues. An attempt to correlate emission and durability to key flow parameters such as flow uniformity peak velocity and velocity index is made. For this purpose, transient flow simulations of a close-coupled (CC) and underbody converter are performed. The study also includes relations between the transient and steady analysis results in order to assess if steady-state CFD is sufficient.

ASSESING CONVERTER DESIGN

FLOW UNIFORMITY INDEX - Flow uniformity index, proposed by Weltens et. al. [1], helps quantify the uniformity of the distribution of flow speed at a cross-section of a catalyst. It is a commonly used criteria in evaluating converter designs. It can be as high as 1 for perfectly uniform flows, and usually values over 0.8 are preferable. Reynolds number is known have a significant influence on the uniformity index, γ, [1]. Today, due to the stringent emission regulations, designs are expected meet higher flow uniformity, typically over 0.90 for underbody and 0.85 for close-coupled configurations.

Martin et. al. [2] studied the influence of flow uniformity on catalyst light-off, ageing and conversion of NOx, CO and HC. They concluded that flow maldistribution does not improve light-off, promotes ageing and degrades conversion capability. Taylor and Ciray [3] quantified the conversion and pressure loss performance of converters as a function of flow uniformity. They concluded that backpressure will double compared to ideal distribution when γ was 0.6. The similar trend of lower conversion at lower γ was also shown by Martin et. al.. Both studies use steady computational modeling.

OTHER PARAMETERS – Several other parameters are often used in evaluating converter performance and durability.

Space Velocity – It relates volumetric exhaust gas flow rate to monolith size. Lower space velocity means longer residence times and hence higher conversion.

Velocity Ratio – Ratio of peak velocity to the mean velocity on catalyst face. It helps determine the range of flow speeds on catalyst. Usually expected to be lower than 2. This criterion is relevant to flow uniformity index.

Velocity Index – Peak velocity location in the normalized coordinate system. It ranges from −1 to 1, 0 being the monolith center. Values under |0.7| (or 70%) are considered acceptable. When the bulk of the gas

contacts the outer part of the brick, there is a higher chance of thermal problems such as mat erosion.

Peak Velocity – It is important in terms of brick erosion. Exhaust gas impacting the catalyst front face faster than 100 m/s may cause brick erosion.

Pressure Drop – Pressure difference across the monolith. Pressure drop is important due to its implications on engine power. It is dictated by catalyst brick geometry but also depends on flow uniformity.

TRANSIENT VERSUS STEADY-STATE APPROACH

Traditionally steady-state analysis of the hot-end flow has been performed in CFD applications due to computer resource and time constraints [4,5]. Typically a transient simulation over the same configuration will require 1-2 orders of more computer time and more importantly an external resource for time dependent boundary conditions. Therefore, there is a significant incentive to use a steady method when it is justified. In steady-state CFD approach different inflow conditions may be used to determine different exhaust system properties. For example, to assess converter washcoat durability and effectiveness, typically each port (i.e. engine cylinder) is fired one by one at a single predetermined condition (e.g. peak engine cycle mass flow). Another analysis may be to calculate backpressure by forcing flow from every exhaust manifold port simultaneously.

Such steady-state approaches produce results that are believed to be reasonable in terms of prediction in an averaged sense (or a worst case sense), and become more valid for underbody converters where pressure pulsations are weaker. However, the current trend for converters is to be placed closer to the engine in order to reduce light-off time. Use of the steady-state approximation for the analysis of close-coupled converters becomes questionable. Therefore, an unsteady approach seems more appropriate when evaluating such designs. Transient CFD methods have recently been used for assessing catalyst light-off performance [6] and exhaust system behavior [7-10].

In a transient simulation the challenge is to obtain accurate time-dependent boundary conditions, i.e. the right mass flow rate and temperature as the crank angle changes. This may be achieved by experimental measurements or via coupling with an engine cycle simulation code. The numerical option is preferable due to the expense and impracticality involved in such an experimental procedure.

However, important questions need to be answered first:

1. Are steady-state results sufficient to evaluate the design? Or should the design be evaluated based on the more detailed information the transient method provides? For underbody converters? For close-coupled converters?

2. Is it practical to use transient information for analysis and design?

3. Which flow parameter(s) are the best in terms of evaluating designs?

This study aims to answer or rather is an initiation to find the answers to these questions. So far, our answers are:

1. Steady-state analysis is adequate for underbody converters since gas pulsations are weaker. However, for close-coupled catalysts the exhaust gas flow rate is a strong function of crank angle.

2. A transient analysis will produce large amount of data, including all flow details at every time step. It is not feasible to just look at the results and offer a better design. Even when key parameters are utilized, they will be a function of time (see Figure 2), which may be hard to digest.

3. The authors believe that flow uniformity index is the single most important parameter that has the best capability of summarizing flow distribution quality on a catalyst section. It has the most implications on emissions and backpressure. Velocity index and peak velocity are valuable complements because they are indicative of durability problems.

Two configurations (one close-coupled and one underbody) with the same set of boundary conditions are scrutinized in order to answer question 1 above. Flow uniformity index, peak velocity and velocity index are the key parameters chosen for this purpose.

A CLOSE-COUPLED CONVERTER

TRANSIENT ANALYSIS - A coupled 1-D/3-D transient analysis of the hot-end flow field for a 1.6L engine had been performed recently by Berkman et. al.[10]. That study had emphasized on assessing the time-dependent flow uniformity variation, determination of a suitable location for O2 sensor, and checking for risk of brick erosion. In the particular study the exhaust manifold and converter had been resolved using CFD (STAR-CD code) and the rest of the system including full intake-engine-exhaust components were modeled by an engine cycle simulation code (WAVE). Two engine speeds were considered, 3000 and 6000 RPM. Further details on the numerical modeling are given in Ref. [10]. Figure 1

shows the discretized close-coupled converter geometry over which the CFD simulations were done.
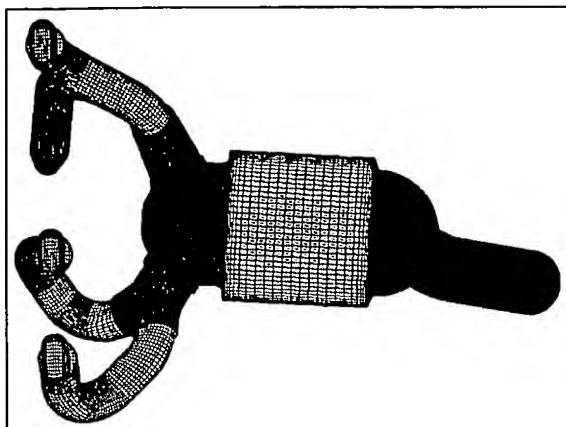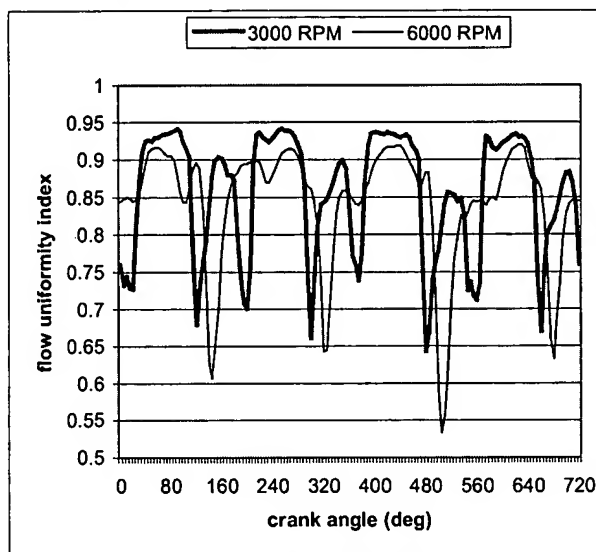

Figure 1: Close-Coupled Converter

Figure 2: Transient Flow Uniformity, Close-Coupled Catalyst

Figure 2 shows the most important set of results for the two transient runs: the variation of flow uniformity index as a function of crank angle during an engine cycle. It shows instants of significantly low γ values (as low as 0.54 for 6000 RPM case) during exhaust blowdown. At these instances, since almost all of the flow is directed on to the catalyst from a single port, the flow is highly maldistributed as shown in Figure 3. Also, here the mass flow rate (thus Reynolds number) is much higher causing even lower flow uniformity. Such dips will occur for any close-coupled design for very brief durations during operation and is very difficult for the designer to eliminate. Also note that for 3000 RPM there are 8 such dips of which only 4 are due to the port firings. A second set of 4 dips (slightly less in severity) occurs quite regularly. They take place at a very low mass flow rate

when none of the ports is active. It basically is a poor velocity distribution on the catalyst due to lack of pressure and exhaust gas at certain instances. This poor value does not result in poor conversion, since the mass flow rate at such instances is more than one order of magnitude less than the average gas flow rate. On the contrary, the poor distribution during the exhaust blowdown is critical since more exhaust gas is present in the converter at such durations. This shows that even the flow uniformity index by itself does not fully relate to emissions or performance. Therefore, while determining a "mean" transient flow uniformity value, the γ values are weighted by the instantaneous mass flow rate associated with them. This is called a "cycle mass average" versus a non-weighted average, i.e. the mean of the curve in Fig. 2, named "cycle average", as presented in Table 1.

Figure 3: Flow Distribution during Port Firings

STEADY ANALYSIS – The same configuration (Fig. 1) was also subjected to a steady-state approach in order to understand the correlation between the two analyses. For the steady-state analysis three different sets of boundary conditions had been used:

1. Cycle averaged mass flow rate shared by all ports
2. Cycle averaged mass flow rate through single port (port 3)
3. Peak mass flow rate through single port (port 3)

Table 1: Flow Uniformity Index

	3000 RPM	6000 RPM
Transient – cycle mass averaged	0.8399	0.8263
Transient – cycle averaged	0.8585	0.8421
Steady – condition 1	0.9215	0.9036
Steady – condition 2	0.9126	0.8739
Steady – condition 3	0.8290	0.8395

Table 1 compares the flow uniformity variation on a case-by-case basis. The tabulated results indicate that transient averages are best approximated by using a worst-case condition (peak cycle mass flow) in the steady-state approach. Obviously, while a steady-state simulation does not provide details as in Fig. 2, it provides a very good feel for the cycle mass averaged flow uniformity.

Table 2: Peak Velocity (m/s)

	3000 RPM	6000 RPM
Transient – overall peak	< 120	< 145
Steady – condition 1	12.4	23.2
Steady – condition 2	25.4	53.6
Steady – condition 3	99.7	87.0

The computed peak gas velocity encountered by the front face of the catalyst is given in Table 2 above. The predicted peak velocity by steady-state method is significantly less than the overall peak velocity captured by transient analysis. Even the worst case (condition 3) underpredicts it by up to 67%.

Velocity index is a parameter that defines the location of peak velocity. However, much like the flow uniformity this parameter is dependent upon the instantaneous mass flow rate in a transient simulation. For example for this particular catalyst it is seen that the velocity index is around 80-90% for long durations when none of the ports are active and the mass flow through the catalyst is minimal. However, during port firings velocity index gets smaller. Latter values bear more significance in terms of durability, and a "threshold velocity weighted" value should be utilized. This is similar to the cycle mass averaging approach used to calculate a mean flow uniformity index. For this particular case the velocity index values are only counted if the peak velocity exceeds 30 m/s on the catalyst front face. Table 3 compares the mean transient velocity index values for 3000 and 6000 RPM cases along with their steady-state counterparts. All the numbers lie within a narrow range. Note that in steady cases 2 and 3, only port 3 is active. Remarkably, these two cases overpredict the velocity index only slightly. Steady-state analysis seems to give reasonably close results to the averaged transient velocity index at both RPMs. Also note that at both RPMs the trends among ports are similar, i.e. port 2 yielding the best peak velocity location. The design is a successful one in terms of velocity index where the peak velocity remains with 70% limit.

For close-coupled converters or maniverters it is obvious that a transient simulation is preferable over steady-state analysis where details are looked over. The peak velocity is significantly underpredicted when steady-state CFD is utilized, which may lead to unexpected brick durability issues. Steady analysis agrees well for flow uniformity and velocity index compared to transient approach.

Table 3: Velocity Index (%)

	3000 RPM	6000 RPM
Transient – all ports threshold aver	52.6	54.6
Transient – port 1 threshold aver	49.8	54.7
Transient – port 2 threshold aver	45.3	49.3
Transient – port 3 threshold aver	56.3	57.2
Transient – port 4 threshold aver	58.3	57.6
Steady – condition 1 all ports	57.2	58.0
Steady – condition 2 port 3	65.2	59.1
Steady – condition 3 port 3	59.1	59.1

AN UNDERBODY CONVERTER

TRANSIENT ANALYSIS – The same engine-out conditions (gas flow rate and temperature) for the 3000 RPM transient case were used as boundary conditions for an underbody converter of the same size. This time the hot-end was replaced with a long straight downpipe going into a generic inlet cone followed by an identical catalyst with a generic outlet cone and exhaust pipe. Such a set-up enables us to compare the performance of an underbody design against the close-coupled configuration. Figure 4 shows the configuration.
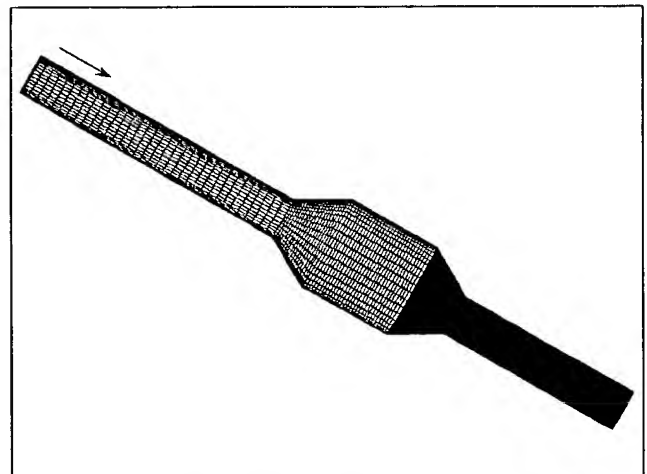

Figure 4: Underbody Converter

The cycle mass averaged flow uniformity value is 0.9510 for the underbody converter. This is a significantly higher value compared to the close-coupled design (0.8399). The main reason is that the underbody configuration has a long straight pipe and a straight inlet cone in front of the catalyst where the flow is allowed to develop into a fully turbulent pipe flow, and is expanded into the brick smoothly. As seen in Figure 1, the close-coupled catalyst hardly enjoys such a favorable design. Four runners merge into a hemispherical mixing bowl that is bounded by the brick on the other end. Obviously, flow will be more concentrated on certain spots based on which port is firing. Figure 5 compares the flow uniformity variation (scale on right side) during an engine cycle at 3000 RPM for the close-coupled and underbody converter locations. The inlet mass flow rate is also included in the plot (scale on left side) that helps understand the correlation between the engine dynamics and the flow distribution over the catalyst. It is seen that the underbody case has better flow distribution on average as discussed, and features 8 dips as well. Note that these dips are shifted in time (crank angle) with respect to their close-coupled counter parts, and are smaller magnitude. The phase shift happens since the underbody catalyst is further downstream. The dips are due to the same mechanisms discussed before. The first set of four due to firing and the next set of four due to consequential poor distribution. However, the duration for these dips, i.e. duration of poor flow distribution is shorter than the close-coupled case as well as less severe. This is an indication that a steady-state analysis may be very effective for underbody converter flow simulation.
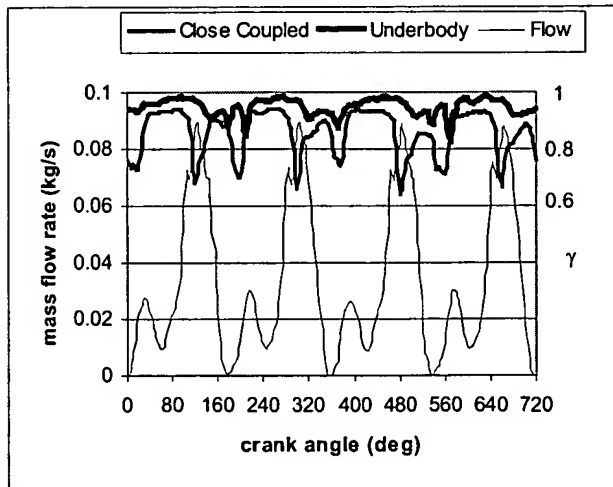

Figure 5: Transient Flow Uniformity, 3000 RPM

STEADY ANALYSIS – The underbody configuration was also subjected to a steady-state analysis in order to understand the correlation between the two analyses. For the steady-state analysis two different sets of boundary conditions had been used:

1. Cycle averaged mass flow rate
2. Instantaneous peak mass flow rate

Table 4 compares the key flow parameters for the transient and steady-state simulations. The steady analysis with cycle averaged condition γ value is higher than its transient counter part, where as the steady analysis – condition 2 (peak mass flow rate) value is in excellent agreement. These follow the trend of the close-coupled converter configuration. The velocity index for underbody catalyst stays firmly within 10%. This indicates that the peak velocity lies in the core of the brick and is an advantage offered by underbody converter designs.

Table 4: Underbody Converter Results

	γ	Peak Velocity (m/s)	Velocity Index
Transient	0.9510 (cycle mass averaged)	< 27	< 10%
Steady – condition 1	0.9753	11.4	9.22 %
Steady – condition 2	0.9507	29.9	9.22 %

The steady-state peak mass flow rate (worst case scenario) case yields a slightly higher peak velocity on the catalyst face compared to the transient analysis. This is notable because for the close-coupled case, the worst condition steady-state analysis significantly underestimates peak velocity. For the close-coupled catalyst, the peak velocity is sensitive to the high engine pulsations. However, since the underbody catalyst is further downstream, the gas has time and space to expand, compress and develop (higher γ) until it reaches the catalyst. Therefore, the underbody catalyst sees much lower magnitudes of peak velocity compared to the close-coupled converter. In the case of steady peak mass flow rate, the amount of mass flow is similar to that of the instantaneous rate in the transient case where the peak is obtained. Therefore, it gives a very good upper bound for peak velocity encountered by the brick. The steady cycle averaged mass flow simulation underpredicts the peak velocity as expected. A steady analysis with the peak mass flow rate is truly effective in providing a worst-case scenario for catalyst performance and durability in this study.

CONCLUSIONS

In brief, based on the configurations studied, for underbody converters steady-state CFD analysis with a worst-case scenario (i.e. peak mass flow rate) is effective for prediction of catalyst flow and performance.

It is suggested to use steady-state approach when possible, because usually a transient CFD analysis will require 1-2 more orders of computational time and resources. Besides, the solver has to be coupled to an engine cycle simulation code, which may not be available or practical.

However, in the case of a close-coupled design where the inlet design is suspect, a transient CFD simulation is very valuable tool to highlight performance and durability issues, and possibly warrant a design change if necessary.

ACKNOWLEDGMENTS

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